Exact Diagonalisation of The XY-Hamiltonian of Open Linear Chains with Periodic Coupling Constants and Its Application to Dynamics of One-Dimensional Spin Systems

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Abstract

A new method of diagonalisation of the XY-Hamiltonian of inhomogeneous open linear chains with periodic (in space) changing Larmor frequencies and coupling constants is developed. As an example of application, multiple quantum dynamics of an inhomogeneous chain consisting of 1001 spins is investigated. Intensities of multiple quantum coherences are calculated for arbitrary inhomogeneous chains in the approximation of the next nearest interactions.

Key words: linear spin chain, nearest–neighbour approximation, three–diagonal matrices, diagonalisation, fermions, multiple–quantum NMR, multiple–quantum coherence, intensities of multiple–quantum coherences.

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1 Introduction

One-dimensional exactly solvable models (spin chains, rings) [1] have been actively employed for studying various problems of spin dynamics [2] and quantum information theory [3]. Substantial progress in our understanding of spin dynamics has been achieved on the basis of a homogeneous XY model for spin chains ($s = 1/2$) in transverse magnetic field [4]. Recently, Hamiltonians of the simplest inhomogeneous systems (alternating systems) have been diagonalised for the ring [5] and the linear spin chain [6]. Development of methods for exact solution of inhomogeneous spin problems has become especially urgent in conjunction with recent progress in quantum computation and quantum information theories [3]. In particular, these methods can be used for studying the quantum state transfer from one end of the chain to another one [7, 8] The qubit addressing problem

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can be attacked by variation of the Larmor frequencies of different spins [9] in classical one-dimensional models. This immediately brings inhomogeneity into the XY model as diagonal elements of the corresponding Hamiltonian are not equal. Consequently, we arrive at one-dimensional spin models with Hamiltonians described by three-diagonal matrices which elements on the diagonal are not-equal, and those under and over the main diagonal are not identically equal as well. Low sensitivity of nuclear magnetic resonance (NMR), which is widely applied in experimental implementation of quantum computations [3], leads to a further complication of the model described above. Consideration of k-qubit systems brings us naturally to the study of $kn + r$ spin chains ($r < k$, n is arbitrary, k, n, r are positive integers), with Larmor frequencies and constants of spin-spin interactions repeating periodically with period k.

The paper suggests a new method of diagonalisation of a Hamiltonian of a linear k-periodic spin chain of length $kn + r$ for various values $r < k$. Special attention is given to the case $k = 3$. For a spin chain of $3n + 2$ sites with periodic parameters (period 3) a multiple quantum dynamics [10, 2] is analysed and intensities of all MQ coherences are calculated (see Figure 2). This analysis is based on the explicit diagonalisation of the Hamiltonian of a linear 3-periodic spin chain with $3n + 2$ sites (Theorem 5.1) and the exact formulae, obtained in the paper (Theorem 6.1), for the intensities of all MQ coherences developed in any nuclear spin system coupled by the nearest neighbour dipolar interactions. We conclude the paper with a discussion of the properties of eigenvalues and eigenvectors of the general k-periodic systems with $kn - 1$ sites (Theorem 7.1).

2 Model

The Hamiltonian of a spin-1/2 open chain with only nearest neighbour (NN) couplings has the following general form

$$H = \sum_{n=1}^{N} \omega_n I_{nz} + \sum_{n=1}^{N-1} D_{n,n+1} \left(I_{n,x} I_{n+1,x} + I_{n,y} I_{n+1,y} \right), \tag{1}$$

where ω_n, $n = 1, ..., N$, are the Larmor frequencies, and $D_{n,n+1}$, $n = 1, ..., N-1$, are the NN coupling constants. The nuclear spins are specified by the spin-1/2 operators $I_{n\alpha}$ at the sites $n = 1, ..., N$ with the projections $\alpha = x, y, z$. The Jordan–Wigner transformation [4]

$$\begin{aligned} I_{n,-} &= I_{n,x} - iI_{n,y} = (-2)^{n-1} \left(\textstyle\prod_{l=1}^{l=n-1} I_{l,z} \right) c_n, \\ I_{n,+} &= I_{n,x} + iI_{n,y} = (-2)^{n-1} \left(\textstyle\prod_{l=1}^{l=n-1} I_{l,z} \right) c_n^+, \\ I_{n,z} &= c_n^+ c_n - 1/2 \end{aligned} \tag{2}$$

from the spin-1/2 operators $I_{n\alpha}$ to the creation (annihilation) operators c_n^+ (c_n) of the spineless fermions takes the Hamiltonian (1) into the Hamiltonian

$$H = \sum_{n=1}^{N} \omega_n \left(c_n^+ c_n - 1/2 \right) + \frac{1}{2} \sum_{n=1}^{N-1} D_{n,n+1} \left(c_n^+ c_{n+1} + c_{n+1}^+ c_n \right), \tag{3}$$

or in the matrix notations into

$$H = \frac{1}{2}\mathbf{c}^{+}\left(D + 2\Omega\right)\mathbf{c} - \frac{1}{2}\sum_{n=1}^{N}\omega_n. \tag{4}$$

In Eq. (4) we denote the row vector $\left(c_1^{+}, ..., c_N^{+}\right)$ by $\mathbf{c}^{+}$, the column vector $(c_1, ..., c_N)^t$ by $\mathbf{c}$ (the superscript 't' represents the transpose), and specify the matrices Ω and D as

$$\Omega = \begin{bmatrix} \omega_1 & 0 & \cdots & 0 & 0 \\ 0 & \omega_1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \omega_{N-1} & 0 \\ 0 & 0 & \cdots & 0 & \omega_N \end{bmatrix}, \quad D = \begin{bmatrix} 0 & D_1 & \cdots & 0 & 0 \\ D_1 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & D_{N-1} \\ 0 & 0 & \cdots & D_{N-1} & 0 \end{bmatrix}. \tag{5}$$

To diagonalise the matrix $D+2\Omega$ means to construct such unitary matrix $U = \{u_{nk}\}_{n,k=1}^{N}$ and diagonal matrix $\Lambda = diag\{\lambda_1, ..., \lambda_N\}$ that

$$D + 2\Omega = U\Lambda U^{+}, \tag{6}$$

where the superscript '+' represents the conjugate transpose, and columns $(u_{1l}, ..., u_{Nl})^t$ of U, $l = 1, ..., N$, form an orthonormal basis of eigenvectors of $H = D + 2\Omega$. The new fermion operators γ_k^{+} and γ_k introduced by the relations

$$c_n^{+} = \sum_{k=1}^{N} u_{nk}^{*}\gamma_k^{+}, \quad c_n = \sum_{k=1}^{N} u_{nk}\gamma_k \tag{7}$$

bring Hamiltonian (4) into the Hamiltonian

$$H = \frac{1}{2}\sum_{k=1}^{N}\lambda_k\gamma_k^{+}\gamma_k - \frac{1}{2}\sum_{n=1}^{N}\omega_n \tag{8}$$

with energies $\lambda_\nu/2$ of the free fermion waves.

The problem of diagonalisation of $D + 2\Omega$ with arbitrary constants ω_n, $n = 1, ..., N$, and D_k, $k = 1, ..., N-1$, for large N ($N \sim 10^6$) and computation of various functions of $D + 2\Omega$ is a time consuming problem usually dealt with the help of super computers. On the other hand, there are two known exact solutions (suitable for studying systems with large N) for such a problem when the spin-system considered has periodic changing Larmor frequencies and coupling constants. Namely, the case of equal sites ($\omega_1 = ... = \omega_n = a$, $D_1 = ... = D_{N-1} = c$) has been solved in [4], while the case of period 2 with odd N ($\omega_1 = \omega_3 = ... = \omega_N$, $\omega_2 = \omega_4 = ... = \omega_{N-1}$, $D_1 = D_3 = ... = D_{N-2}$, $D_2 = D_4 = ... = D_{N-1}$) has been solved in [6]. The present paper concerns properties of a general periodic chain. In the following sections we shall demonstrate how to reduce the diagonalisation problem of the Hamiltonian of a k-periodic chain with $kn - 1$ sites ($k > 2, n > 1$) to the problem

of finding roots for explicitly given polynomials of degree less or equal k. Therefore, the methods developed are particularly useful when $n >> k$.

In what follows we will utilise essentially the result on diagonalisation of the homogeneous (in other words, 1-periodic) chain [4] which we state now.

Lemma 2.1 *Let $c \neq 0$, then the matrix*

$$J_n(a,c) = \begin{bmatrix} a & c & 0 & \cdots & 0 & 0 & 0 \\ c & a & c & \cdots & 0 & 0 & 0 \\ 0 & c & a & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & a & c & 0 \\ 0 & 0 & 0 & \cdots & c & a & c \\ 0 & 0 & 0 & \cdots & 0 & c & a \end{bmatrix} \tag{9}$$

has n-distinct eigenvalues

$$\lambda_j = a + 2c \cdot cos\left(\frac{\pi j}{n+1}\right), \quad j = 1, ..., n, \tag{10}$$

and the corresponding eigenvectors are of the form

$$\vec{x}_j = \left(sin\left(\frac{\pi j}{n+1}\right), sin\left(\frac{2\pi j}{n+1}\right), ..., sin\left(\frac{n\pi j}{n+1}\right)\right). \tag{11}$$

Proof. It is a straightforward verification.

3 Reduction over the Period

Let us consider an open periodic chain of $kn + d$ sites ($k > d \geq 0$, $k > 1$) with k-periodic non–zero NN coupling constants:

$$D_1 = D_{k+1} = ... = D_{kn+1}, \quad \cdots \quad D_d = D_{k+d} = ... = D_{kn+d},$$

$$D_{d+1} = D_{k+d+1} = ... = D_{k(n-1)+d+1}, \quad \cdots \quad D_k = D_{2k} = ... = D_{kn}, \tag{12}$$

and k-periodic Larmor frequencies

$$\omega_1 = \omega_{k+1} = ... = \omega_{kn+1}, \quad \cdots \quad \omega_d = \omega_{k+d} = ... = \omega_{kn+d},$$

$$\omega_{d+1} = \omega_{k+d+1} = ... = \omega_{k(n-1)+d+1}, \quad \cdots \quad \omega_k = \omega_{2k} = ... = \omega_{kn}, \tag{13}$$

($D_i, \omega_j \in \mathbb{R}$, $D_i \neq 0$, $i, j = 1, ..., k$). We shall demonstrate how to reduce the diagonalisation problem for the Hamiltonian of such a system to the problem of diagonalising of a certain $k \times k$ block matrix which entries are matrices of dimension $m \times m$, $(m+1) \times (m+1)$,

$m \times (m+1)$ and $(m+1) \times m$ ($m = n$ in Section 5 and $m = n-1$ in Section 7). A particular case of this reduction will be used in the consecutive sections for studying k-periodic chains of length $kn-1$.

Before we proceed we make an agreement regarding our notations. If a Gothic letter is used in the description of any matrix as its element, then this means that the corresponding place in the matrix is a matrix. The size and the structure of a matrix denoted by a Gothic letter should be clear or given in the context. Therefore, the original matrix is a block matrix. To underline that the matrix consists of blocks we shall often denote such matrices in bold. We shall also denote by I_m the $m \times m$ identity matrix.

The Hamiltonian of a k-periodic system with $kn+d$ sites has the following form:

$$H = D + 2\Omega, \tag{14}$$

where

$$\Omega = \begin{bmatrix}
\omega_1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\
0 & \omega_2 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & \omega_{k-1} & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & \cdots & 0 & \omega_k & 0 & \cdots & 0 & 0 & \cdots & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 & \omega_1 & \cdots & 0 & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & \omega_k & 0 & \cdots & 0 & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \omega_1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & \omega_{d-1} & 0 \\
0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & 0 & \cdots & 0 & \omega_d
\end{bmatrix} \tag{15}$$

and

$$D = \begin{bmatrix}
0 & D_1 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\
D_1 & 0 & D_2 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\
0 & D_2 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & D_{k-1} & 0 & \cdots & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & \cdots & D_{k-1} & 0 & D_k & \cdots & 0 & \cdots & 0 & 0 \\
0 & 0 & 0 & \cdots & 0 & D_k & 0 & \cdots & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & D_{d-1} \\
0 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \cdots & D_{d-1} & 0
\end{bmatrix}. \tag{16}$$

To diagonalise matrix H one finds (real) eigenvectors u_ν and (real) eigenvalues λ_ν, $\nu = 1$, ... $kn+d$, which satisfy the following equation

$$(D + 2\Omega)u_\nu = \lambda_\nu u_\nu. \tag{17}$$

To resolve this equation we associate to each vector $u \in \mathbb{R}^{kn+d}$ vectors $u_{(j)}$, $j = 1, ..., k$, formed by those coordinates of u whose numbers have residue j modulo k. Observe that among vectors $u_{(1)}, ..., u_{(k)}$ there are d-vectors of dimension $(n+1)$ and $(k-d)$ vectors of dimension n. Now equation (17) can be rewritten as a system of n linear equations in $u_{(j)}$:

$$\mathbf{H} \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = \lambda_\nu \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} \tag{18}$$

with matrix $\mathbf{H} = 2\mathbf{\Omega} + \mathbf{D}$. Here

$$\mathbf{\Omega} = \begin{bmatrix} \mathcal{W}_1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \mathcal{W}_2 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \mathcal{W}_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \mathcal{W}_{k-1} & 0 \\ 0 & 0 & 0 & \cdots & 0 & \mathcal{W}_k \end{bmatrix}, \tag{19}$$

$\mathcal{W}_j = \omega_j I_{n+1}$ for $j = 1, ..., d$, $\mathcal{W}_j = \omega_j I_n$ for $j = d+1, ..., k$, and with an exception of two degenerate cases

$$\mathbf{D} = \begin{bmatrix} 0 & \mathcal{D}_1 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & \mathcal{D}_k^t \\ \mathcal{D}_1 & 0 & \mathcal{D}_2 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & \mathcal{D}_2 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & \mathcal{D}_{d-1} & 0 & \mathcal{D}_d^t & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & \mathcal{D}_d & 0 & \mathcal{D}_{d+1} & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & \mathcal{D}_{d+1} & 0 & \mathcal{D}_{d+2} & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & \ddots & \ddots & \mathcal{D}_{k-2} & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \ddots & 0 & \mathcal{D}_{k-1} \\ \mathcal{D}_k & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & \cdots & \mathcal{D}_{k-1} & 0 \end{bmatrix}, \tag{20}$$

with $\mathcal{D}_j = D_j I_{n+1}$ for $j = 1, 2, ..., d-1$, $\mathcal{D}_j = D_j I_n$ for $j = d+1, ..., k-1$, and $\mathcal{D}_d, \mathcal{D}_k : \mathbb{R}^{n+1} \to \mathbb{R}^n$ given by

$$\mathcal{D}_d = \begin{bmatrix} D_d & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & D_d & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_d & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & D_d & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & D_d & 0 \end{bmatrix}, \qquad \mathcal{D}_k = \begin{bmatrix} 0 & D_k & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_k & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & D_k & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & D_k \end{bmatrix}. \tag{21}$$

It is easy to see that

$$\mathcal{D}_d\mathcal{D}_d^t = D_d^2 I_n, \qquad \mathcal{D}_k\mathcal{D}_k^t = D_k^2 I_n, \qquad \mathcal{D}_d\mathcal{D}_k^t = D_d D_k J_n^t, \qquad \mathcal{D}_k\mathcal{D}_d^t = D_k D_d J_n, \tag{22}$$

where J_n is the Jordan $n \times n$ cell:

$$J_n = \begin{bmatrix} 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & 1 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}. \tag{23}$$

There are two degenerate cases. In the case $k = 2$ matrix $\mathbf{D}$ decomposes as

$$\mathbf{D} = \begin{bmatrix} 0 & \mathcal{L}^t \\ \mathcal{L} & 0 \end{bmatrix} \tag{24}$$

where $\mathcal{L} : \mathbb{R}^{n+d} \to \mathbb{R}^n$:

$$\mathcal{L} = \begin{bmatrix} D_1 & D_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & D_1 & D_2 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_1 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & \ddots & \ddots \end{bmatrix}, \tag{25}$$

while in the case $k > 2$ and $d = 0$ we do not get matrix $\mathcal{D}_d$ and matrix $\mathcal{D}_k : \mathbb{R}^n \to \mathbb{R}^n$ is of the form

$$\mathcal{D}_k = \begin{bmatrix} 0 & D_k & 0 & \cdots & 0 & 0 \\ 0 & 0 & D_k & \cdots & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & D_k \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}. \tag{26}$$

It is easy to see that this matrix satisfies $\mathcal{D}_k\mathcal{D}_k^t = D_k^2 I_{n-1,1}$ for a diagonal matrix $I_{n-1,1}$ with the first $n-1$ diagonal elements equal to 1 and the last one equals to 0.

Remark 3.1 *From the reduction obtained above we divide consideration of the diagonalisation problem into three different cases: period $k = 2, 3$ and $k \geq 4$. In each case there are further reductions depending on the value of d. In the next sections we shall work out the case $k \geq 3$ and $d = k - 1$.*

4 Some Auxiliary Results

The diagonalisation process of Sections 5 and 7 will relay on some elementary facts about matrices of the form $H_{i,j} - \lambda I_{j-i+1}$ where for $i < j$:

$$H_{i,j} = \begin{bmatrix} 2\omega_i & D_i & 0 & \cdots & 0 & 0 \\ D_i & 2\omega_{i+1} & D_{i+1} & \cdots & 0 & 0 \\ 0 & D_{i+1} & 2\omega_{i+2} & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2\omega_{j-1} & D_{j-1} \\ 0 & 0 & 0 & \cdots & D_{j-1} & 2\omega_j \end{bmatrix}. \tag{27}$$

These facts are mostly know and we give their proofs only for the reader's convenience.

Lemma 4.1 *If $D_s \neq 0$ for all $s = i, ..., j-1$, then all the eigenvalues of the matrix $H_{i,j}$ are distinct.*

Proof. Under the assumption that all D_s, $s = i, ..., j$, are non–zero, one can reconstruct every eigenvector u_ν of $H_{i,j}$ by its eigenvalue λ_ν and the first coordinate u_1. Moreover, the expressions for all other coordinates u_s, $s = 2, ..., j-i+1$, of u_ν are linear in u_1. This implies that every two eigenvectors u_ν and u'_ν with the same eigenvalue λ_ν are proportional with coefficient u_1/u'_1.

Lemma 4.2 *Non-diagonal elements of the adjoint matrix of $(H_{i,j} - \lambda I_{j-i+1})$ are*

$$\mathrm{adj}_{s,t}\left\{(H_{i,j} - \lambda I_{j-i+1})\right\} = \mathrm{adj}_{t,s}\left\{(H_{i,j} - \lambda I_{j-i+1})\right\} =$$

$$= (-1)^{s+t} det\left(H_{i,i+s-2} - \lambda I_{s-1}\right) D_{i+s-1} \cdots D_{i+t-2} det\left(H_{i+t,j} - \lambda I_{j-i-t+1}\right) \tag{28}$$

where the first index in $\mathrm{adj}_{s,t}\{\cdot\}$ denotes the row number, the second denotes the column number and $t > s$. The diagonal elements of the adjoint matrix are

$$\mathrm{adj}_{s,s}\left\{(H_{i,j} - \lambda I_{j-i+1})\right\} = det\left(H_{i,i+s-1} - \lambda I_{s-1}\right) det\left(H_{i+s+1,j} - \lambda I_{j-i-s}\right). \tag{29}$$

Proof. The first part follows from an observation that element D_{i+s-2} situated in row $(s-1)$ and column s of matrix $(H_{i,j} - \lambda I_{j-i+1})$ does not contribute to the cofactor (s,t) of $(H_{i,j} - \lambda I_{j-i+1})$, and similarly for element D_{i+t-1} situated in row t and column $(t+1)$. The second part is due to the splitting of the complement to the element (s,s) of $(H_{i,j} - \lambda I_{j-i+1})$ into $(H_{i,i+s-1} - \lambda I_{s-1})$ and $(H_{i+s+1,j} - \lambda I_{j-i-s})$.

Corollary 4.1 *If we denote elements of $(H_{i,j} - \lambda I_{j-i+1})^{-1}$ by $P_{s,t}$ (s — row, t — column), then for $t > s$*

$$P_{t,s} = P_{s,t} = (-1)^{s+t} \frac{det\left(H_{i,i+s-2} - \lambda I_{s-1}\right) D_{i+s-1} \cdots D_{i+t-2} det\left(H_{i+t,j} - \lambda I_{j-i-t+1}\right)}{det\left(H_{i,j} - \lambda I_{j-i+1}\right)}. \tag{30}$$

The diagonal terms $P_{t,t}$ are

$$P_{t,t} = \frac{det\left(H_{i,i+t-1} - \lambda I_{t-1}\right) det\left(H_{i+t+1,j} - \lambda I_{j-i-t}\right)}{det\left(H_{i,j} - \lambda I_{j-i+1}\right)}. \tag{31}$$

Lemma 4.3 *If $D_1 \neq 0$, then matrices $H_{1,k}$ and $H_{2,k}$ ($k \geq 2$) have no common eigenvalues.*

Proof. First, observe that it is true for $k = 2$:

$$det\,(H_{1,2} - \lambda I_2) = (2\omega_1 - \lambda) \cdot (2\omega_2 - \lambda) - D_1^2, \tag{32}$$

and if λ is a root of $det\,(H_{2,2} - \lambda I_1) = 0$, then $\lambda = 2\omega_2$, which is the root of

$$(2\omega_1 - \lambda) \cdot (2\omega_2 - \lambda) - D_1^2 = 0 \tag{33}$$

only if $D_1 = 0$.

For general k, if λ is a root of

$$det\,(H_{2,k} - \lambda I_{k-1}) = 0, \tag{34}$$

then for such λ:

$$det\,(H_{1,k} - \lambda I_k) = (2\omega_1 - \lambda) det\,(H_{2,k} - \lambda I_{k-1}) - D_1^2 det\,(H_{3,k} - \lambda I_{k-2}) =$$

$$= -D_1^2 det\,(H_{3,k} - \lambda I_{k-2})\,. \tag{35}$$

For the last polynomial we can assume that it is non zero by inductive hypothesis and because $D_1 \neq 0$. From here the statement follows.

5 Exact Diagonalisation for a Spin Chain with $3n + 2$ Sites

To demonstrate how the reduction over the period works, first we study a partial case of the main result, namely a chain of period 3 with $3n + 2$ sites. The reduction of Section 3 leads us to the following system of linear equations:

$$\begin{bmatrix} 2\mathcal{W}_1 - \lambda_\nu I_{n+1} & \mathcal{D}_1 & \mathcal{D}_3^t \\ \mathcal{D}_1 & 2\mathcal{W}_2 - \lambda_\nu I_{n+1} & \mathcal{D}_2^t \\ \mathcal{D}_3 & \mathcal{D}_2 & 2\mathcal{W}_3 - \lambda_\nu I_n \end{bmatrix} \begin{bmatrix} u_{(1)} \\ u_{(2)} \\ u_{(3)} \end{bmatrix} = 0. \tag{36}$$

Remind that $\mathcal{W}_j$, $j = 1, 2, 3$, are just scalar matrices, as well as the matrix $\mathcal{D}_1$, while $\mathcal{D}_2, \mathcal{D}_3 : \mathbb{R}^{n+1} \to \mathbb{R}^n$ are given below:

$$\mathcal{D}_2 = \begin{bmatrix} D_2 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 0 & D_2 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_2 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & D_2 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & D_2 & 0 \end{bmatrix}, \qquad \mathcal{D}_3 = \begin{bmatrix} 0 & D_3 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 0 & D_3 & \cdots & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & D_3 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & D_3 \end{bmatrix}. \tag{37}$$

From the second equation of (36)

$$(\lambda_\nu - 2\omega_2) \cdot u_{(2)} = \mathcal{D}_1 u_{(1)} + \mathcal{D}_2^t u_{(3)}. \tag{38}$$

Assume that an eigenvalue λ_ν of H is not equal to $2w_2$, then

$$u_{(2)} = \frac{D_1}{\lambda_\nu - 2\omega_2} \cdot u_{(1)} + \frac{1}{\lambda_\nu - 2\omega_2} \cdot \mathcal{D}_2^t u_{(3)}. \tag{39}$$

Substituting $u_{(2)}$ into the first equation and into the third equation of (36), and using that $\mathcal{D}_2\mathcal{D}_2^t = D_2^2 I_n$ we obtain a system:

$$\begin{cases} \left(D_1^2 - (\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)\right) u_{(1)} + \left(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right) u_{(3)} = 0, \\ \left((\lambda_\nu - 2\omega_2)\mathcal{D}_3 + D_1\mathcal{D}_2\right) u_{(1)} + \left(D_2^2 - (\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3)\right) u_{(3)} = 0. \end{cases} \tag{40}$$

Lemma 5.1 *If*

$$(\lambda_\nu - 2\omega_1)\,(\lambda_\nu - 2\omega_2) \neq D_1^2, \tag{41}$$

then the following inequality holds

$$(\lambda_\nu - 2\omega_2)\,(\lambda_\nu - 2\omega_3) \neq D_2^2. \tag{42}$$

Proof. Observe, that if $\lambda_\nu = 2\omega_2$, then

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) = 0 \neq D_1^2 \tag{43}$$

and

$$(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_1) = 0 \neq D_2^2. \tag{44}$$

Therefore, it is left to consider the case when $\lambda_\nu \neq 2\omega_2$. Assume that

$$(\lambda_\nu - 2\omega_2)\,(\lambda_\nu - 2\omega_3) = D_2^2. \tag{45}$$

Then from the second equation of (40)

$$\left((\lambda_\nu - 2\omega_2)\mathcal{D}_3 + D_1\mathcal{D}_2\right) u_{(1)} = 0. \tag{46}$$

With respect to the standard scalar product $\langle\cdot,\cdot\rangle_{\mathbb{R}^m}$, $m = n, n+1$, we have:

$$0 = \langle u_{(3)}, \left((\lambda_\nu - 2w_2)\mathcal{D}_3 + D_1\mathcal{D}_2\right) u_{(1)}\rangle_{\mathbb{R}^n} = \langle \left(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right) u_{(3)}, u_{(1)}\rangle_{\mathbb{R}^{n+1}}. \tag{47}$$

Therefore, in order to satisfy the first equation of (40) we necessarily have

$$\begin{cases} \left(D_1^2 - (\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)\right) u_{(1)} = 0, \\ \left(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right) u_{(3)} = 0. \end{cases} \tag{48}$$

From here and under the assumption that

$$(\lambda_\nu - 2\omega_1)\,(\lambda_\nu - 2\omega_2) \neq D_1^2, \tag{49}$$

we obtain that $u_{(1)} = 0$. Because $D_j \neq 0$, $j = 1, 2, 3$, the matrix

$$\left(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\right) \tag{50}$$

has rank n and its kernel is 0. Therefore, $u_{(3)} = 0$. Finally, from (39) we obtain that $u_{(2)} = 0$ and thus, λ_ν is not an eigenvalue for H. This verifies the lemma.

Assume as in Lemma 5.1 that

$$(\lambda_\nu - 2\omega_1)\,(\lambda_\nu - 2\omega_2) \neq D_1^2, \tag{51}$$

then from the first equation of (40) we deduce that

$$u_{(1)} = \frac{D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\,\mathcal{D}_3^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2}u_{(3)}. \tag{52}$$

Substituting (52) into (39) we obtain

$$u_{(2)} = \frac{(\lambda_\nu - 2\omega_1)\mathcal{D}_2^t + D_1\mathcal{D}_3^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2}u_{(3)}. \tag{53}$$

Due to Lemma 5.1

$$(\lambda_\nu - 2\omega_2)\,(\lambda_\nu - 2\omega_3) \neq D_2^2. \tag{54}$$

Thus, from the second equation of (40) we have that

$$u_{(3)} = \frac{(\lambda_\nu - 2\omega_2)\,\mathcal{D}_3 + D_1\mathcal{D}_2}{(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - D_2^2}u_{(1)}. \tag{55}$$

Therefore, because $\lambda_\nu \neq 2\omega_2$, $u_{(3)}$ satisfies

$$\left((\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - (\lambda_\nu - 2\omega_3)D_1^2 - (\lambda_\nu - 2\omega_1)D_2^2 - (\lambda_\nu - 2\omega_2)D_3^2\right)u_{(3)} =$$

$$= \left(D_1\mathcal{D}_3\mathcal{D}_2^t + D_1\mathcal{D}_2\mathcal{D}_3^t\right)u_{(3)}. \tag{56}$$

This leads us to the following theorem:

Theorem 5.1 *For $j = 1, ..., n$ each of the three solutions of the cubic equation*

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - (\lambda_\nu - 2\omega_2)D_3^2 - (\lambda_\nu - 2\omega_1)D_2^2 - (\lambda_\nu - 2\omega_3)D_1^2 =$$

$$= 2D_1D_2D_3cos\left(\frac{\pi j}{n+1}\right) \tag{57}$$

is an eigenvalue for H. The component $u_{(3)}$ of the corresponding eigenvector u_ν is

$$u_{(3)} = \left(sin\left(\frac{\pi j}{n+1}\right), sin\left(\frac{2\pi j}{n+1}\right), ..., sin\left(\frac{n\pi j}{n+1}\right)\right). \tag{58}$$

The remaining components $u_{(1)}$ and $u_{(2)}$ are determined uniquely from

$$u_{(1)} = \frac{(\lambda_\nu - 2\omega_2)\,\mathcal{D}_3^t + D_1\mathcal{D}_2^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2} u_{(3)}, \tag{59}$$

and

$$u_{(2)} = \frac{(\lambda_\nu - 2\omega_1)\mathcal{D}_2^t + D_1\mathcal{D}_3^t}{(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) - D_1^2} u_{(3)}. \tag{60}$$

where $\mathcal{D}_2$, $\mathcal{D}_3$ are given in (37).
There are two other eigenvalues of H which satisfy the following quadratic equation

$$(\lambda_\nu - 2\omega_1)\,(\lambda_\nu - 2\omega_2) - D_1^2 = 0. \tag{61}$$

The component $u_{(3)}$ of the corresponding eigenvector u_ν is necessarily zero, the component $u_{(1)}$ spans the (one-dimensional) kernel of

$$(\lambda_\nu - 2\omega_2)\mathcal{D}_3 + D_1\mathcal{D}_2 \tag{62}$$

and the component $u_{(2)}$ is

$$u_{(2)} = \frac{D_1}{\lambda_\nu - 2\omega_2} \cdot u_{(1)}. \tag{63}$$

All eigenvalues constructed are distinct and they exhaust all $3n+2$ distinct eigenvalues for H.

Proof. Let us consider the case when $2w_2$ is an eigenvalue for H and u_ν is the corresponding eigenvector. Then for the components $u_{(1)}$ and $u_{(3)}$ we have from the second equation of (36):

$$u_{(1)} = -\frac{1}{D_1} \cdot \mathcal{D}_2^t u_{(3)}. \tag{64}$$

From the first equation of (36):

$$u_{(2)} = -\frac{1}{D_1}\left(\frac{2\omega_2 - 2\omega_1}{D_1} \cdot \mathcal{D}_2^t + \mathcal{D}_3^t\right) u_{(3)}. \tag{65}$$

Substituting this into the third equation of (36) we obtain:

$$\left(-\frac{1}{D_1} \cdot \mathcal{D}_3\mathcal{D}_2^t + -\frac{1}{D_1}\left(\frac{2\omega_2 - 2\omega_1}{D_1} \cdot \mathcal{D}_2\mathcal{D}_2^t + \mathcal{D}_2\mathcal{D}_3^t\right) + (2\omega_3 - 2\omega_2)\right) u_{(3)} =$$

$$= \left((2\omega_3 - 2\omega_2) - (2\omega_2 - 2\omega_1)\frac{D_2^2}{D_1^2} - \frac{D_2 D_3}{D_1}(J_n + J_n^t)\right) u_{(3)} = 0. \tag{66}$$

Thus, from Lemma 2.1

$$2(\omega_3 - \omega_2)D_1^2 + 2(\omega_1 - \omega_2)D_2^2 - 2D_1 D_2 D_3 cos\left(\frac{\pi j}{n+1}\right) = 0 \tag{67}$$

for some $j = 1, ..., n$. From here it follows that $2\omega_2$ also satisfies Eq. (57), moreover, the formulae for the component $u_{(3)}$ and (as a consequence) for $u_{(1)}$ and $u_{(2)}$ coincide with those given in the body of the theorem. We obtain that the case $\lambda_\nu = 2\omega_2$ can be considered simultaneously with all the other solutions of (57).

Therefore, every eigenvalue for H is either a solution for

$$(\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2) = D_1^2, \tag{68}$$

or it is a solution of (57) for some $j = 1, ..., n$. Because H has exactly $3n + 2$ eigenvalues and all of them are distinct (see Lemma 4.1), all the solutions of the quadratic equation and of n cubic equations are multiplicity free and pairwise distinct.

Now the first part of Theorem 5.1 follows from the remarks above, from (56) and Lemma 2.1. Indeed if (56) admits a nontrivial solution for some λ_ν, then either $\lambda_\nu = 2\omega_2$ or

$$\mu = \big((\lambda_\nu - 2\omega_1)(\lambda_\nu - 2\omega_2)(\lambda_\nu - 2\omega_3) - (\lambda_\nu - 2\omega_3)D_1^2 - (\lambda_\nu - 2\omega_1)D_2^2 - (\lambda_\nu - 2\omega_2)D_3^2\big) \tag{69}$$

is an eigenvalue for $D_1\mathcal{D}_3\mathcal{D}_2^t + D_1\mathcal{D}_2\mathcal{D}_3^t$. The first case has been already discussed, while for the second we apply Lemma 2.1. It follows then that μ is necessarily of the form

$$2D_1D_2D_3 cos\left(\frac{\pi j}{n+1}\right) \tag{70}$$

for some $j = 1, ..., n$. As it was explained before, among those $3n$ eigenvalues constructed there are no repeated. The component $u_{(3)}$ of the corresponding eigenvectors are uniquely determined by the eigenvalues due to Lemma 2.1. The other two components $u_{(1)}$ and $u_{(2)}$ are also uniquely determined by (52) and (53) respectively. This gives us a unique eigenvector u_ν of H for each solution of (57).

The second part of the statement follows from (40) because

$$\big(D_1\mathcal{D}_2^t + (\lambda_\nu - 2\omega_2)\mathcal{D}_3^t\big) \tag{71}$$

has rank n and its kernel is 0.

6 Multiple Quantum Spin Dynamics of an Inhomogeneous Spin Chain with $3n + 2$ Sites

Information on the exact spectrum of the Hamiltonian of an open spin chain provides us with the techniques for determining the multi-quantum dynamics in such a system. The MQ NMR dynamics of the nuclear spins coupled by the nearest neighbour dipolar interactions was developed in [2]. The corresponding Hamiltonian is

$$H_{MQ} = \frac{1}{2}\sum_{n=1}^{N-1} D_{n,n+1}\{I_{n,+}I_{n+1,+} + I_{n,-}I_{n+1,-}\}. \tag{72}$$

The Hamiltonian H_{MQ} (72) takes exactly the form of the Hamiltonian H (1) with the Larmor frequencies $\omega_n = 0$ for all the sites, by making use of the unitary transformation [12]

$$Y = exp\left(-i\pi I_{2,x}\right) exp\left(-i\pi I_{4,x}\right) \cdots exp\left(-i\pi I_{N-1,x}\right) \tag{73}$$

acting on the even sites so that $YH_{MQ}Y^{+} = H$ (Eq. (1); $\{\omega_n = 0\}$). The transformation Y brings the initial density matrix at the high temperature approximation (see [11] for details):

$$\rho(0) = \sum_{j=1}^{N} I_{j,z} = \sum_{j=1}^{N} \left(c_j^{+} c_j - 1/2\right) \tag{74}$$

to the form

$$\bar{\rho}(0) = Y I_z Y^{+} = \sum_{n=1}^{N} (-1)^{n-1} I_{n,z}, \tag{75}$$

where we introduce the total polarisation $I_z = \sum_{n=1}^{N} I_{n,z}$. The Liouville–von Neumann equation ($\hbar = 1$)

$$i\frac{\partial \rho}{\partial t} = [H_{MQ}, \rho] \tag{76}$$

with the Hamiltonian H_{MQ} (72) and the initial density matrix $\rho(0)$ (74) gives us the intensities $G_n(t)$ of $n = 0$ and $n = \pm 2$ orders only with the conservation conditions [12, 13]

$$G_0(t) + G_2(t) + G_{-2}(t) = 1. \tag{77}$$

Theorem 6.1 *The intensity $G_n(t)$, $n = 0, \pm 2$, of MQ coherences of the Hamiltonian H_{MQ} (72) are*

$$G_0(t) = \frac{Tr\left[\cos^2\left(H_{MQ} \cdot t\right)\right]}{N}, \quad G_{\pm 2}(t) = \frac{Tr\left[\sin^2\left(H_{MQ} \cdot t\right)\right]}{2N}. \tag{78}$$

Proof. According to [9]

$$G_2(t) = G_{-2}(t) = \frac{1}{N} \sum_{k=1,3,\ldots} \sum_{n=2,4,\ldots} \left| \sum_{j=1}^{N} (-1)^j S_{jk} S_{jn}^{*} \right|^2, \tag{79}$$

with

$$S_{jk} = \sum_{l} u_{jl}^{*} u_{kl} e^{-\frac{i}{2}\lambda_l t}, \tag{80}$$

where λ_l are the eigenvalues of H_{MQ}, $l = 1, ..., N$, and the unitary matrix $U = \{u_{kl}\}_{k,l=1}^{N}$ diagonalises H_{MQ}. Let us rewrite (79) in the matrix form:

$$G_2(t) = G_{-2}(t) = \frac{1}{N} Tr\left(B_0 A B_1 A^{*}\right), \tag{81}$$

where B_0 is the diagonal matrix with ones in odd rows and zeroes in even rows, B_1 is the diagonal matrix with ones in even rows and zeroes in odd rows:

$$B_0 = diag\{1, 0, 1, 0, ...\}, \quad B_1 = diag\{0, 1, 0, 1, ...\};$$

and the matrix A is

$$A = S\left(B_1 - B_0\right)S^*, \quad S = exp\left(-\frac{i}{2}H_{MQ}\cdot t\right). \tag{82}$$

Observe that

$$\left(B_1 - B_0\right)H_{MQ} = -H_{MQ}\left(B_1 - B_0\right). \tag{83}$$

Therefore,

$$\left(B_1 - B_0\right)\cdot S\cdot\left(B_1 - B_0\right) = S^* \quad \text{and} \quad Tr\left[(S)^m\right] = Tr\left[(S^*)^m\right]. \tag{84}$$

Using

$$AA^* = A^2 = I_N, \quad A\left(B_1 - B_0\right)A^* = \left(B_1 - B_0\right)(S^*)^4 \tag{85}$$

and

$$Tr\left[A\left(B_1 - B_0\right)A^*\right] = Tr\left[\left(B_1 - B_0\right)A^*A\right] = Tr\left[\left(B_1 - B_0\right)AA^*\right] \tag{86}$$

we deduce

$$Tr\left[B_0AB_1A^*\right] = \frac{1}{4}Tr\left[\left(I - \left(B_1 - B_0\right)\right)A\left(I + \left(B_1 - B_0\right)\right)A^*\right] =$$

$$= \frac{1}{4}Tr\left[AA^* - \left(B_1 - B_0\right)AA^* + A\left(B_1 - B_0\right)A^* - \left(B_1 - B_0\right)A\left(B_1 - B_0\right)A^*\right] =$$

$$= \frac{1}{4}Tr\left[I_N - (S^*)^4\right] = -\frac{1}{8}Tr\left[S^4 + (S^*)^4 - 2I_N\right] =$$

$$= \frac{1}{2}Tr\left[\left(\frac{S^2 - (S^*)^2}{2i}\right)^2\right] = \frac{1}{2}Tr\left[\sin^2\left(H_{MQ}\cdot t\right)\right]. \tag{87}$$

From here the result follows.

Remark 6.1 *In [6] Formula (78) was proposed for alternating spin chains. Theorem 6.1 establishes the same formula for arbitrary spin chains coupled by the nearest neighbour dipolar interactions.*

Theorem 6.1 together with Theorem 5.1 allow us to calculate MQ coherence intensities of the zero and the second orders, $G_0(t)$ and $G_2(t) + G_{-2}(t)$, without performing matrix multiplication, by solving $O(N)$ cubic equations (compare with [9]). Let us consider a linear spin chain of length 1001 which consists of four-spin fragments represented in Figure 1.

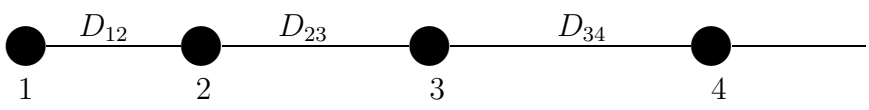

Figure 1. The four–spin fragment of the linear chain. The distances between neighbouring spins in the fragments are 2.7, 3 and 3.3 $\dot{A}$. The dipolar coupling constants are $D_{12} = 2\pi 6096$, $D_{23} = 2\pi 4444$, $D_{34} = 2\pi 3339 s^{-1}$.

The distances between neighbouring spins in the fragments are $2.7\dot{A}$, $3\dot{A}$ and $3.3\dot{A}$. The dipolar coupling constants $D_{12} = 2\pi 6096$, $D_{23} = 2\pi 4444$, $D_{34} = 2\pi 3339 s^{-1}$ are used in all numerical calculations. The intensities of MQ coherences for the inhomogeneous linear chain with $N = 1001$ spins consisting of fragments of Figure 1 are shown in Figure 2. The dynamics behaviour coincides with the one given in [9].

7 The Generalisation of the Method for Spin Chains with $kn - 1$ Sites

Now we consider the case of a k-periodic system with $kn - 1$-sites. According to Section 3, to diagonalise Hamiltonian of such a system we have to solve the following system of linear equations

$$\mathbf{H} \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = \lambda_\nu \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix}, \tag{88}$$

where

$$\mathbf{H} = \begin{bmatrix} & & & & & \mathcal{D}_k^t \\ & & & & & 0 \\ & & \mathcal{H}_{1,k-1} & & & \vdots \\ & & & & & 0 \\ & & & & & \mathcal{D}_{k-1}^t \\ \mathcal{D}_k & 0 & \cdots & 0 & \mathcal{D}_{k-1} & 2\mathcal{W}_k \end{bmatrix}, \tag{89}$$

and

$$\mathcal{H}_{1,k-1} = \begin{bmatrix} 2\mathcal{W}_1 & \mathcal{D}_1 & 0 & \cdots & 0 & 0 \\ \mathcal{D}_1 & 2\mathcal{W}_2 & \mathcal{D}_2 & \cdots & 0 & 0 \\ 0 & \mathcal{D}_2 & 2\mathcal{W}_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2\mathcal{W}_{k-2} & \mathcal{D}_{k-2} \\ 0 & 0 & 0 & \cdots & \mathcal{D}_{k-2} & 2\mathcal{W}_{k-1} \end{bmatrix}. \tag{90}$$

Observe that because all $\mathcal{D}_j$, $j = 1, ..., k-2$, are diagonal $n \times n$ matrices, it is also true that

$$\mathcal{H}_{1,k-1} = H_{1,k-1} \otimes I_n. \tag{91}$$

Assume λ_ν is not an eigenvalue for $\mathcal{H}_{1,k-1}$ (equivalently, is not an eigenvalue for $H_{1,k-1}$), and consider the matrix

$$\mathbf{G} = \begin{bmatrix} & & & 0 \\ & \left(\mathcal{H}_{1,k-1} - \lambda_\nu I_{n(k-2)}\right)^{-1} & & \vdots \\ & & & 0 \\ 0 & \cdots & 0 & I_{n-1} \end{bmatrix}. \tag{92}$$

Under the above assumption on λ_ν the eigenvector equation

$$\mathbf{H}\begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = \lambda_\nu \begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} \tag{93}$$

is equivalent to

$$\mathbf{G}\left(\mathbf{H} - \lambda_\nu I_{nk-1}\right)\begin{bmatrix} u_{(1)} \\ \vdots \\ u_{(k)} \end{bmatrix} = 0, \tag{94}$$

or in another form to

$$\begin{bmatrix} 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 1 \\ \mathcal{D}_k & 0 & \cdots & 0 & \mathcal{D}_{k-1} \end{bmatrix} \mathbf{G} \begin{bmatrix} \mathcal{D}_k^t \\ 0 \\ \vdots \\ 0 \\ \mathcal{D}_{k-1}^t \\ 2\mathcal{W}_k - \lambda_\nu I_{n-1} \end{bmatrix} \Bigg] \Bigg] \begin{bmatrix} u_{(1)} \\ u_{(2)} \\ \vdots \\ u_{(k-2)} \\ u_{(k-1)} \\ u_{(k)} \end{bmatrix} = 0. \tag{95}$$

Let us denote elements of the matrix $\left(H_{1,k-1} - \lambda_\nu I_{k-1}\right)^{-1}$ by $P_{i,j}$ (i — row, j — column). Using

$$\left(\mathcal{H}_{1,k-1} - \lambda_\nu I_{n(k-1)}\right)^{-1} = \left(H_{1,k-1} \otimes I_n - \lambda_\nu I_{k-1} \otimes I_n\right)^{-1} = \left(H_{1,k-1} - \lambda_\nu I_{k-1}\right)^{-1} \otimes I_n,$$

we derive from (93) for $k-1 \geq j \geq 1$ that

$$u_{(j)} = -\left(P_{j,1} \cdot \mathcal{D}_k^t + P_{j,k-1} \cdot \mathcal{D}_{k-1}^t\right) u_{(k)}. \tag{96}$$

Substituting this expression with $j = 1$ and $j = k-1$ into the last equation of (93) we obtain:

$$\left(P_{1,1} \cdot \mathcal{D}_k\mathcal{D}_k^t + P_{1,k-1}\mathcal{D}_k\mathcal{D}_{k-1}^t + P_{k-1,1} \cdot \mathcal{D}_{k-1}\mathcal{D}_k^t + P_{k-1,k-1} \cdot \mathcal{D}_{k-1}\mathcal{D}_{k-1}^t\right) u_{(k)} =$$

$$= \left(2\omega_k - \lambda_\nu\right) u_{(k)}. \tag{97}$$

Because

$$\mathcal{D}_{k-1}\mathcal{D}_{k-1}^t = D_{k-1}^2 I_{n-1}, \quad \mathcal{D}_k\mathcal{D}_k^t = D_k^2 I_{n-1}, \quad \mathcal{D}_{k-1}\mathcal{D}_k^t = D_{k-1}D_k J_{n-1}^t,$$

$$\mathcal{D}_k\mathcal{D}_{k-1}^t = D_{k-1}D_k J_{n-1}, \tag{98}$$

with the help of Corollary 4.1 we derive that if λ_ν is not an eigenvalue of $H_{1,k-1}$, then the component $u_{(k)}$ of the corresponding eigenvector u_ν belongs to the kernel of

$$\mathcal{M} = \left(det\left(H_{2,k-1} - \lambda_\nu I_{k-2}\right) D_k^2 + det\left(H_{1,k-2} - \lambda_\nu I_{k-2}\right) D_{k-1}^2 -\right.$$

$$-(2\omega_k - \lambda_\nu)det\left(H_{1,k-1} - \lambda_\nu I_{k-2}\right)) \cdot I_{n-1} + (-1)^k D_1 \cdots D_k \left(J_{n-1} + J_{n-1}^t\right). \tag{99}$$

Since

$$(2\omega_k - \lambda_\nu)det\left(H_{1,k-1} - \lambda_\nu I_{k-2}\right) - det\left(H_{1,k-2} - \lambda_\nu I_{k-2}\right) D_{k-1}^2 = det\left(H_{1,k} - \lambda_\nu I_k\right)$$

we can simplify the expression for $\mathcal{M}$:

$$\mathcal{M} = \left(det\left(H_{2,k-1} - \lambda_\nu I_{k-2}\right) D_k^2 - det\left(H_{1,k} - \lambda_\nu I_k\right) D_{k-1}^2\right) \cdot I_{n-1} +$$

$$+(-1)^k D_1 \cdots D_k \left(J_{n-1} + J_{n-1}^t\right). \tag{100}$$

Therefore,

$$\left(det\left(H_{1,k} - \lambda_\nu I_k\right) D_{k-1}^2 - det\left(H_{2,k-1} - \lambda_\nu I_{k-2}\right) D_k^2\right) u_{(k)} =$$

$$= (-1)^k D_1 \cdots D_k \left(J_{n-1} + J_{n-1}^t\right) u_{(k)}. \tag{101}$$

We are ready to state the main result of the paper.

Theorem 7.1 *Each eigenvalue of the Hamiltonian H of a k-periodic system with $kn-1$ sites is either an eigenvalue of $H_{1,k-1}$ or it is a solution of the equation*

$$det\left(H_{1,k} - \lambda_\nu I_k\right) - det\left(H_{2,k-1} - \lambda_\nu I_{k-2}\right) D_k^2 = (-1)^k 2 D_1 \cdots D_k cos\left(\frac{\pi j}{n}\right), \tag{102}$$

for some $j = 1, ..., n-1$. Equation (102) does not have repeated roots and all $k(n-1)$ solutions constructed from (102) are pairwise distinct and are not eigenvalues for $H_{1,k-1}$.

If λ_ν is the solution of (102) for some $j = 1, ..., n-1$, then it is an eigenvalue for H and the component $u_{(k)}$ of the corresponding eigenvector u_ν is

$$u_{(k)} = \left(sin\left(\frac{\pi j}{n}\right), \ldots, sin\left(\frac{(n-1)\pi j}{n}\right)\right). \tag{103}$$

The other components $u_{(j)}$, $j = 1, ..., k-1$, are determined uniquely from

$$u_{(j)} = \frac{(-1)^{j-1}}{det\left(H_{1,k-1} - \lambda_\nu I_{k-1}\right)} \cdot \left[D_1 \cdots D_{j-1} det\left(H_{j+1,k-1} - \lambda_\nu I_{k-j-1}\right) \cdot \mathcal{D}_k^t +\right.$$

$$\left. +(-1)^{k-1} det\left(H_{1,j-1} - \lambda_\nu I_{j-1}\right) D_j \cdots D_{k-2} \mathcal{D}_{k-1}^t\right] u_{(k)}, \tag{104}$$

where $\mathcal{D}_{k-1}$, $\mathcal{D}_k$ are given in (21) ($d = k-1$). Every eigenvalue λ_ν of $H_{1,k-1}$ is an eigenvalue of H. The component $u_{(k)}$ of the corresponding eigenvector u_ν of H is zero. The component $u_{(1)}$ spans the one–dimensional kernel of

$$(-1)^{k-1} D_1 \cdots D_{k-2} \mathcal{D}_{k-1} - det\left(H_{2,k-1} - \lambda_\nu I_{k-2}\right) \mathcal{D}_k. \tag{105}$$

The remaining components $u_{(j)}$, $j = 2, ..., k-1$, are

$$u_{(j)} = (-1)^{j-1} \frac{D_1 \cdots D_{j-1} det\left(H_{j+1,k-1} - \lambda_\nu I_{k-j-1}\right)}{det\left(H_{2,k-1} - \lambda_\nu I_{k-2}\right)} u_{(1)}. \tag{106}$$

Proof. The first part of the theorem follows from Lemma 2.1 because H has exactly $kn-1$ distinct eigenvalues. Indeed, if an eigenvalue λ_ν of H is not an eigenvalue of $H_{1,k-1}$, then as it was shown above, the component $u_{(k)}$ of the corresponding eigenvector u_ν of H satisfies (101). Therefore, λ_ν satisfies (102) for some $j=1,...,n-1$.

For the second part of the theorem we again use Lemma 2.1. The component $u_{(k)}$ of the corresponding eigenvector u_ν, satisfies (101), and, therefore, is uniquely determined by λ_ν as stated in Lemma 2.1. The remaining components of the eigenvectors $u_{(\nu)}$ corresponding to the solutions of (102) can be reconstructed from (96) using Corollary 4.1.

Finally, for the last part we observe that from Lemma 4.2 and the property of the adjoint matrix

$$D_{j-1}(-1)^{j-2}\frac{D_1\cdots D_{j-2}det\left(H_{j,k-1}-\lambda_\nu I_{k-j}\right)}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}+$$

$$+\left(2\omega_j-\lambda_\nu\right)(-1)^{j-1}\frac{D_1\cdots D_{j-1}det\left(H_{j+1,k-1}-\lambda_\nu I_{k-j-1}\right)}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}+$$

$$+D_j(-1)^j\frac{D_1\cdots D_j det\left(H_{j+2,k-1}-\lambda_\nu I_{k-j-2}\right)}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}=$$

$$=D_{j-1}\cdot\frac{\mathrm{adj}_{1,j-1}\left\{\left(H_{1,k-1}-\lambda_\nu I_{k-1}\right)\right\}}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}+\left(2\omega_j-\lambda_\nu\right)\cdot\frac{\mathrm{adj}_{1,j}\left\{\left(H_{1,k-1}-\lambda_\nu I_{k-1}\right)\right\}}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}+$$

$$+D_j\cdot\frac{\mathrm{adj}_{1,j+1}\left\{\left(H_{1,k-1}-\lambda_\nu I_{k-1}\right)\right\}}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}=\delta_{1,j}\frac{det\left(H_{1,k-1}-\lambda_\nu I_{k-1}\right)}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}=0, \tag{107}$$

where $k-1>j>1$ and $\delta_{i,j}$ is the Kronecker symbol. We also have

$$D_{k-2}(-1)^{k-3}\frac{D_1\cdots D_{k-3}\left(2\omega_{k-1}-\lambda_\nu\right)}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}+\left(2\omega_{k-1}-\lambda_\nu\right)(-1)^{k-2}\frac{D_1\cdots D_{k-2}}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}=0. \tag{108}$$

If λ_ν is an eigenvalue for $H_{1,k-1}$, then

$$2\omega_1+D_1(-1)\frac{D_1 det\left(H_{3,k-1}-\lambda_\nu I_{k-2}\right)}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}=\frac{det\left(H_{1,k-1}-\lambda_\nu I_{k-2}\right)}{det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)}=0. \tag{109}$$

Therefore, if $u_{(1)}$ spans the kernel of

$$(-1)^{k-1}D_1\cdots D_{k-2}\mathcal{D}_{k-1}-det\left(H_{2,k-1}-\lambda_\nu I_{k-2}\right)\mathcal{D}_k \tag{110}$$

and $u_{(k)}=0$, then vector u_ν with the other components given by (106) does satisfy the eigenvalue equation

$$\left(H-\lambda I_{kn-1}\right)u_\nu=0. \tag{111}$$

This completes the proof.

8 Conclusion

In the paper we proposed a new one-dimensional exactly solvable model for a linear k-periodic (in space) open spin chain with $kn-1$ sites. For the diagonalisation procedure it is important that the number of sites is $(k-1)(\mathrm{mod}k)$. Nevertheless, the model can serve as a good approximation for any linear periodic spin system if the number of sites in it is much more than the period.

The developed method of diagonalisation of the XY-Hamiltonian of inhomogeneous linear spin chains can be applied to different problems of quantum information theory [3,7,8] and spin dynamics. This method allows us to avoid matrix multiplications which are time consuming operations in the systems with large numbers of spins. In some cases we can suggest analytical methods for problems of spin dynamics instead of the known numerical ones [9].

The suggested method could also be applied to different physical and technical problems which use three–diagonal matrices [14]. In particular, new numerical methods of solving such problems could be worked out on the basis of the approach proposed in the paper.

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